

GC×GC-TOFMS for the comparison between different tobacco mainstream smoke

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Tobacco smoke is an extremely complex and dynamic aerosol consisting of liquid/solid droplets (particulate phase) suspended in a mixture of gases and semi-volatiles (gaseous phase). It is formed during overlapping processes of burning, pyrolysis, pyrosynthesis, distillation, sublimation, condensation, filtration and elution¹. Smoke is emitted either as the mainstream smoke inhaled by the smoker or emitted from the smoldering cigarette in the form of sidestream smoke. Mainstream smoke consists of about 5600 identified compounds² and some reports claim the number of unidentified compounds might reach up to 100 000³.

Mainstream tobacco smoke has been analyzed by means of comprehensive two-dimensional gas chromatography coupled to time of flight mass spectrometry (GC×GC-TOFMS), which is an established analytical technique for the characterization of complex mixtures of volatiles. Samples were analyzed after dynamic headspace (DHS) extraction and thermal desorption (TD).

Recently, the chromatographic method was optimized and a procedure was developed to identify large numbers of compounds present in the DHS extract. Over 1800 compounds were tentatively identified and manually classified into chemical component categories according to Rodgman and Perfetti⁴.

Current research focuses on the development of a strategy for the analysis of large numbers of samples from different tobacco formulations. Efforts are directed to the estimation of the relative importance of intra-product variation compared to inter-product variation, to evaluate how powerful the technique is for distinguishing quantitative or qualitative differences between samples. The Statistical Compare (SC) feature of the LECO ChromaTOF[®] software is used for highlighting possible significant variations inside specific classes of compounds.

¹ Liu, C., McAdam, K., Perfetti, T., *Mini-Reviews in Organic Chemistry*, 8 (2011) 349.

² Perfetti T.A, Rodgman A. *Beitr. Tabakforsch. Int.* 24/5 (2011) 215.

³ Wakeham, H. In *162nd National Meeting, American Chemical Society*; Schmeltz, I., Ed.; Plenum Press: Washington, DC, 1971, p 1.

⁴ Rodgman A, Perfetti T.A. *The chemical components of tobacco and tobacco smoke*, CRC Press, 2009.